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THE UNIMOLECULAR OZONE DECOMPOSITION REACTION.(U)
AUG 79 J M HEIMERL, T P COFFEE
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K sub 1 (M = O3)

20. ABSTRACT (Continue on reverse side if necessary and identify by block number) (clt)

After critical examination of available data taken from the literature, we have derived an expression for the unimolecular decomposition reaction $k_1(M{=}O_3) = 4.31 \times 10^{14} \exp(-22.2/RT)$ $cm^3\ mole^{-1}\ s^{-1}$, $300 \le T \le 3000$ K.

10 to the 14th power   cu cm/(mole s), 300 < or = T < or =

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I. INTRODUCTION

We have recently developed a one-dimensional, premixed, laminar flame code that considers detailed elementary reactions and detailed transport properties[1]. As a test of this code we elected to examine the ozone flame, since its flame speed has been measured[2] over the range 17 to 100 mole % ozone. The reactions are

$$O_3 + M \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} O_2 + O + M \qquad (1)$$

$$O + O_3 \underset{k_{-2}}{\overset{k_2}{\rightleftarrows}} O_2 + O_2 \qquad (2)$$

and

$$O + O + M \underset{k_{-3}}{\overset{k_3}{\rightleftarrows}} O_2 + M. \qquad (3)$$

As expected, the most important reaction for our flame studies proved to be reaction (1). Since adiabatic flame temperatures range from 1027 K to 2677 K[2], we required a rate expression for reaction (1) valid over this temperature range.

In 1968 these reactions were reviewed in detail by Johnston[3]. He found that k_1 $(M = O_3) = 9.94 \times 10^{14} \exp(-22.72/RT)$ cm^3 $mole^{-1}$ s^{-1} over the temperature range 200-1000 K. In 1976 the Leeds group[4] recommended his value. (The value for R here is taken as 1.9872 kcal $mole^{-1}$ K^{-1}. To convert to SI units note that 4.184 joules = 1 calorie.)

The only data in the temperature range ~ 600-1000 K available to Johnston were those of Jones and Davidson[5]. All other direct measurements of reaction (1) used by Johnston lay in the range 303-559 K, with most of these taken at temperatures less than 400 K[3].

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1. *J. M. Heimerl and T. P. Coffee, to be published.*

2. *A. G. Streng and A. V. Grosse, "The Ozone to Oxygen Flame," Sixth Symposium (International) on Combustion, Reinhold Publishing Co., 1957, pp 264-273.*

3. *H. S. Johnston, "Gas Phase Reaction Kinetics of Neutral Oxygen Species", NSRDS-NBS20, September 1968.*

4. *D. L. Baulch, D. D. Drysdale, J. Duxbury and S. J. Grant, "Evaluated Kinetic Data for High Temperature Reactions", Butterworths, Boston, 1976, Vol. 3.*

5. *W. M. Jones and N. Davidson, J. Am. Chem. Soc. 84, 2868-2878, 1962.*

Several investigators, all using shock tubes, found indications that the Arrhenius expression for reaction (1) given by Jones and Davidson[5] might not be valid at higher temperatures. Over a combined temperature range of 1340-3300 K, Wray[6] and Kiefer and Lutz[7,8] found their experimental results were consistent with values of k_1/k_2 that were much lower than those predicted using the Jones and Davidson expression. Michael[9] used Benson and Axworthy's[10] value for k_2 and found that his values for k_1 lay progressively lower than those obtained by assuming the Jones and Davidson expression to be valid over the range $\sim$ 1000-1400 K. Finally Center and Kung[11] showed experimental evidence that this rate coefficient is about a factor of two smaller than the value obtained by assuming that Johnston's expression is valid at 3000 K.

The expressions of Johnston and of Jones and Davidson describe the temperature dependence of k_1 over a limited range. Sufficient information seemed to be available to arrive at a better description of the temperature dependence of reaction (1). The data of Michael[9] and the high temperature data of Center and Kung[12] proved to be in a form that made this possible. A complete listing of the low temperature data compiled by Johnson[3], essentially his Table XVIII, and that of Michael[9] is listed in Appendix A. The data of Center and Kung[12] are listed in Appendix B.

II. ANALYSIS

A. General

We desired values for k_1 extending from 300-3000 K so that a valid fit (i.e. Arrhenius description) could be obtained. We should like to use as much of Michael's data and of Center and Kung's data as possible to extend the temperature range covered in Johnston's review. To this end we first examined the dependence of Michael's data for k_1 upon the

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6. *K. L. Wray, J. Chem. Phys. 38, 1518-1524 (1963).*

7. *J. H. Kiefer and R. W. Lutz, J. Chem. Phys. 42, 1709-1714 (1965).*

8. *J. H. Kiefer and R. W. Lutz, "The Effect of Oxygen Atoms on the Vibrational Relaxation of Oxygen", Proceedings of 11th Symposium (International) on Combustion, August 1966, Combustion Institute, PA, 1967, pp 67-76.*

9. *J. V. Michael, J. Chem. Phys 54, 4455-4459 (1971).*

10. *S. W. Benson and A. E. Axworthy, J. Chem. Phys. 42, 2614-2615 (1965).*

11. *R. E. Center and R. T. V. Kung, J. Chem. Phys. 62, 801-807 (1975).*

12. *R. T. V. Kung, priviate communication, 1978.*

value of k_2 and then determined appropriate high temperature values for k_1 from the data of Center and Kung.

In evaluating both the data of Michael and of Center and Kung we have followed Johnston and have converted each of their measurements to equivalent ozone. To do so we have used $k_1 (M=Ar)/k_1(M=Kr) = 1.25$ (ref. 9) and $k_1 (M=O_3)/k_1(M=Ar) = 4.0$ (ref. 3) and have assumed that these ratios are independent of temperature. Should quantitative third body efficiencies as a function of temperature become available and be found to differ significantly from the values we have employed, the analysis presented below would have to be repeated using appropriately adjusted data.

B. Michael's Data

Michael[9] operated his shock tube at low initial pressures (~ 0.04 - 0.2 atmospheres) and large amounts (~ 95%) of krypton as a diluent and so the only reactions of importance are (1) and (2). This leads to the following rate equations:

$$d[O_3]/dt = - k_1[O_3][M] - k_2[O_3][O] \tag{4}$$

and

$$d[O]/dt = + k_1[O_3][M] - k_2[O_3][O]. \tag{5}$$

When the oxygen atom concentration reaches the steady state; i.e., $d[O]/dt = 0$, we can write

$$d[O_3]/dt = - 2 k_1[O_3][M]. \tag{6}$$

Reactions (1) and (2) were modeled by Michael and the logarithm of the calculated ozone concentration was plotted against time. He found no significant deviation from first order kinetics, and k_1 was described by equation (6). However, he had used Benson and Axworthy's value[10] for $k_2 = 3.37 \times 10^{13} \exp(-5.70/RT)$ cm^3 mole^{-1} s^{-1}. Later expressions of Johnston[3], $k_2 = 1.20 \times 10^{13} \exp(-4.79/RT)$ cm^3 mole^{-1} s^{-1} (200-1000 K), and the Leeds group[4], $k_2 = 5.2 \times 10^{12} \exp(-4.15/RT)$ cm^3 mole^{-1} s^{-1} (200-500 K) lead to smaller values for k_2. This means that the time for the oxygen atom concentration to reach steady state will take longer than in Michael's calculations. The question is: how much longer?

We have numerically intergrated equations (4) and (5) for Michael's conditions using the smallest value[4] for k_2 and found that $d[O]/dt \approx 0$ is still valid in the time frame of Michael's experiment, typically 50 to 350 μsec. (Rate coefficients derived using equation (6) will tend to be systematically low but the error is less than ∿ 10%). Note that we must assume that the expression for k_2 is valid up to ∿ 1400 K. This approach appears to be reasonable since Michael's data are not very sensitive to the precise value of k_2.

In summary we find that the later, lower values of k_2 do not significantly affect Michael's results.

C. Center and Kung's Data

Center and Kung[11] operated their shock tube at very low initial pressures (∿ 7×10^{-4} to 3×10^{-2} atmospheres) with a high (95-99%) argon diluent. The time scale of these measurements is tens of microseconds, much shorter than the time scale in Michael's experiment. A simple analytical unfolding of their ozone concentration relaxation time observations could be made provided that $[O] \approx 0$ or more precisely that $k_2\ [O] << k_1\ [M]$. Under these conditions

$$d[O_3]/dt = -k_1\ [M]\ [O_3]. \tag{7}$$

Numerical integration of equations (4) and (5) for their experimental conditions shows that as one progresses from 2000 K to lower temperatures the more important the term involving atomic oxygen becomes (see Equation 4), and that for temperatures greater than 2000 K, the loss rate of ozone can be approximately described by equation (7). In this manner fourteen points of Center and Kung[12] were determined to be valid representations of k_1 and are listed in Table I. A complete listing of their data and a more detailed analysis of their data may be found in Appendix B.

The question remains: what is the sensitivity of these values of k_1 as listed in Table I to the value of k_2? It can be seen in equation (4) that the larger the value of k_2 the more important that term becomes. Here we have used Hampson's[13] expression for $k_2 = 1.14 \times 10^{13} \exp(-4.57/RT)\ cm^3\ mole^{-1}\ s^{-1}$ (200-1000 K). Again this expression for k_2 has been assumed to be valid at the higher temperatures. To test the sensitivity of the values of k_1 on the value of k_2 we have arbitrarily multiplied Hampson's expression for k_2 by two for the 2041 K case (see Table I). We have found that the computed ozone relaxation time (i.e., k_1) changes by about 10%. For the higher temperatures the change is less.

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13. R. F. Hampson, ED., J. Phys. and Chem. Ref. Data 2, 267-308 (1973).

TABLE I. HIGH TEMPERATURE VALUES OF k_1 FROM CENTER AND KUNG

T(K)	k_1 (M = Ar)
2041	5.31(11)*
2128	9.48(11)
2273	1.54(12)
2353	1.76(12)
2439	1.18(12)
2500	9.98(11)
2564	1.08(12)
2564	1.30(12)
2632	1.37(12)
2667	1.62(12)
2703	1.84(12)
2778	2.25(12)
2857	2.24(12)
2941	1.90(12)

*Read as 5.31×10^{11} cm^3 $mole^{-1}$ s^{-1}.

D. The Least Squares Fit

The data can be divided into four groups by temperature: the lower temperature values[3] (303-359 K); the Jones and Davidson[3,5] values, (769-910 K); Michael's[9] values (971-1384 K); and Center and Kung's[11] values, (2041-2941 K). So that the preponderance of low temperature data points would not bias the fit, each group of data was weighted equally. For example, we used 14 values of k_1 from Center and Kung (see Table I) and in this group each value was weighted by 1/14. To avoid biasing the fit toward the higher absolute values of k_1, errors between the least squares fit and the data points were all measured in a relative sense. This is accomplished by using a weight for each value of k_1 equal to the square of the reciprocal of that value. This weight is in addition to the weighting discussed above. The logarithmic method with proper transformation of the weights[14] was used to fit the data points to the two parameter Arrhenius form: $A \exp(-E/RT)$, where $R=1.9872 \times 10^{-3}$ kcal mole^{-1} K^{-1} and T is the temperature. The value k_1 ($M=O_3$) = $4.31 \times 10^{14} \exp(-22.2/RT)$ cm^3 mole^{-1} s^{-1} was found. The number of digits carried is a measure of the precision of the fit and not of the accuracy of the experiments. A listing of the least squares fitting routine coded in FORTRAN for use on a CDC-7600 can be found in Appendix C.

Table II shows the average error for the points in each of the four data groups relative to our recommended fit. The average error for all the data points is also shown. The fact that the average relative error for each data group is comparable to the error in the overall fit is another indication that the fit is not dominated by any single data group. The size of the errors can be traced to the large amount of scatter in the data.

To check the consistency of these independent data and the robustness of the derived two parameter Arrhenius expression, fits were also made by deleting one group of data at a time. These results are given in Table III. The evaluation of these two parameters is seen to be independent of any single data group. Specifically, if the highest temperature data of Center and Kung are deleted, the subsequent expression for k_1 extrapolated to 2500 K yields values only 2% greater than all the data combined. Similarly if Michael's data are deleted the subsequent interpolated value of this expression for k_1 is 17% greater than all the data combined.

Separate fits were made to each of the four data groups. In some cases the parameters so obtained differed markedly from those obtained using all the data. This comes as no surprise since each of the four groups encompass a rather limited temperature range, while taken together they span a temperature range of about a factor of ten.

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14. *R. J. Cvetanovic and D. L. Singleton, Internat. J. of Chem. Kin.* **9**, *481-488, 1977. See also, R. J. Cvetanovic and D. L. Singleton, Internat. J. of Chem. Kin* **9**, *1007-1009, 1977.*

TABLE II. COMPARISON OF DATA FROM EACH GROUP WITH OUR RECOMMENDED FIT

Data Group	Average Relative Error
Low Temp	25%
Jones & Davidson	43%
Michael	41%
Center & Kung	25%
All Data	33%

TABLE III. LEAST SQUARES FIT FOR ALL DATA EXCLUDING DATA GROUPS ONE BY ONE

All Data Except	Log A	E(kcal/mole)
Low Temp	14.39	20.6
Jones & Davidson	14.60	22.2
Michael	14.70	22.3
Center & Kung	14.64	22.2
All Data	14.63	22.2

A three parameter fit of the data was found to yield the expression $k_1 = 5.31 \times 10^{16}\, T^{-0.61} \exp(-23.1/RT)$ $cm^3\, mole^{-1}\, s^{-1}$. The activation energy is about the same as the two parameter case and the average error for all the data in this case is 31%, slightly smaller than the two parameter case. The three parameter fit is sensitive to data deletion and thus we feel that the data are not sufficiently precise to support such a fit. The two parameter fit is essentially just as accurate.

Figure 1a, b, and c show a plot of all the data together with both the two parameter fit (solid line) and the three parameter fit (dashed line) to these data. Since the vertical scale spans about 15 powers of ten, the plot has been segmented into three sections.

For $T \sim 3000$ K the two parameter expression we have derived leads to values of k_1 that are about a factor of two lower than those obtained by assuming that the Johnston expression is valid. Because the Jones and Davidson data constituted the highest temperature available to him, Johnston necessarily weighted his fit heavily toward these data. However, as can be seen in the figure, our expression yields values for k_1 that lie below all the Jones and Davidson data. We do not know if the Jones and Davidson measurements are systematically too high[15], or if there is actually some pre-exponential temperature dependence in the function representing k_1 that cannot yet be discerned because the data are not sufficiently accurate.

ACKNOWLEDGEMENT

We thank R. T. Kung for generously supplying his data. We also thank R. D. Anderson for his help with the figure.

15. *For a discussion of some data reduction problems, see H. B. Palmer, Combustion and Flame 11, 120-124, 1967.*

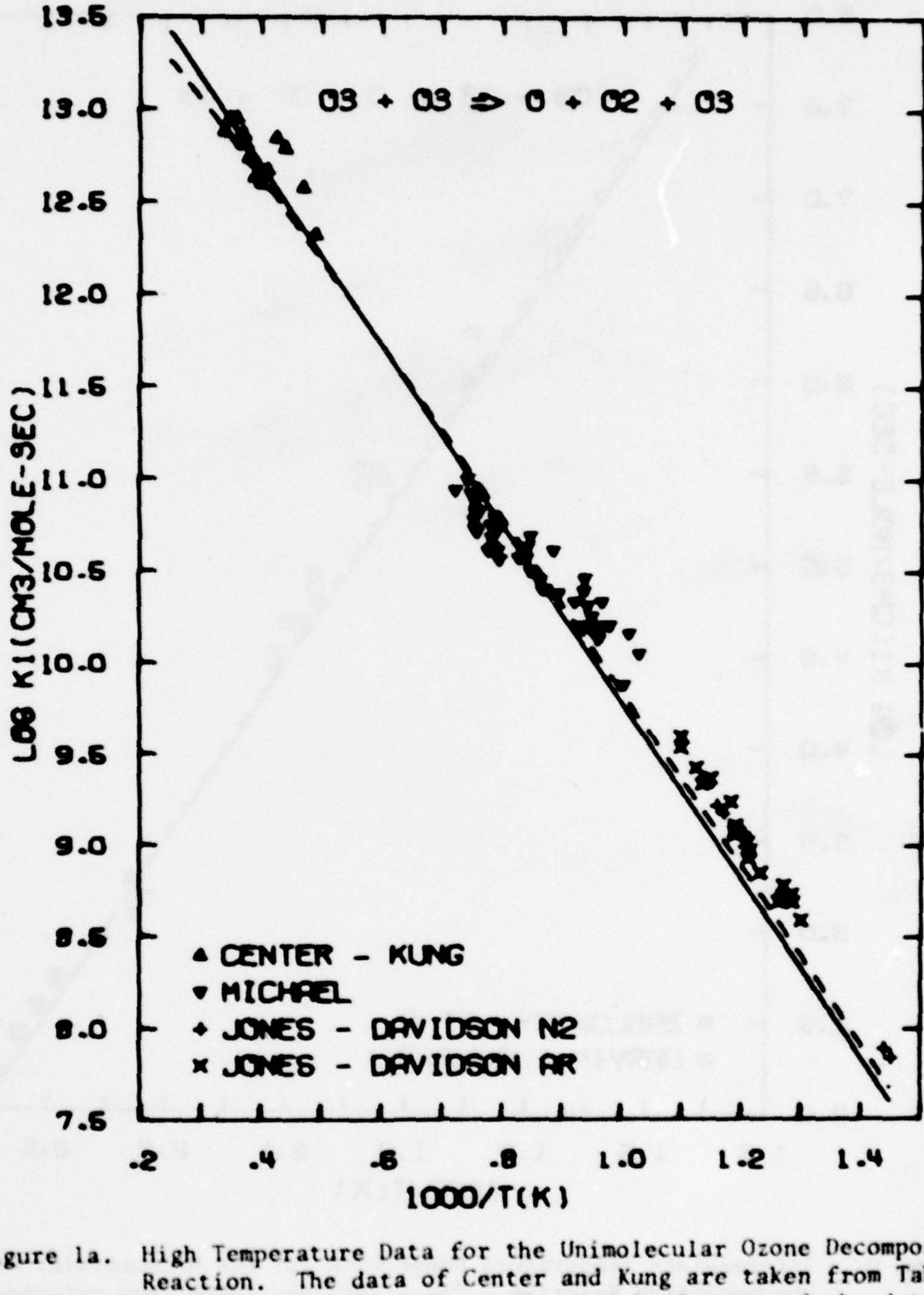

Figure 1a. High Temperature Data for the Unimolecular Ozone Decomposition Reaction. The data of Center and Kung are taken from Table I, the data of Michael from reference 9 of text and the data of Jones and Davidson from reference 3 of text. The data in the figure have been adjusted for M = O_3. The solid and dashed lines show respectively the best two and three parameter fits to all the data.

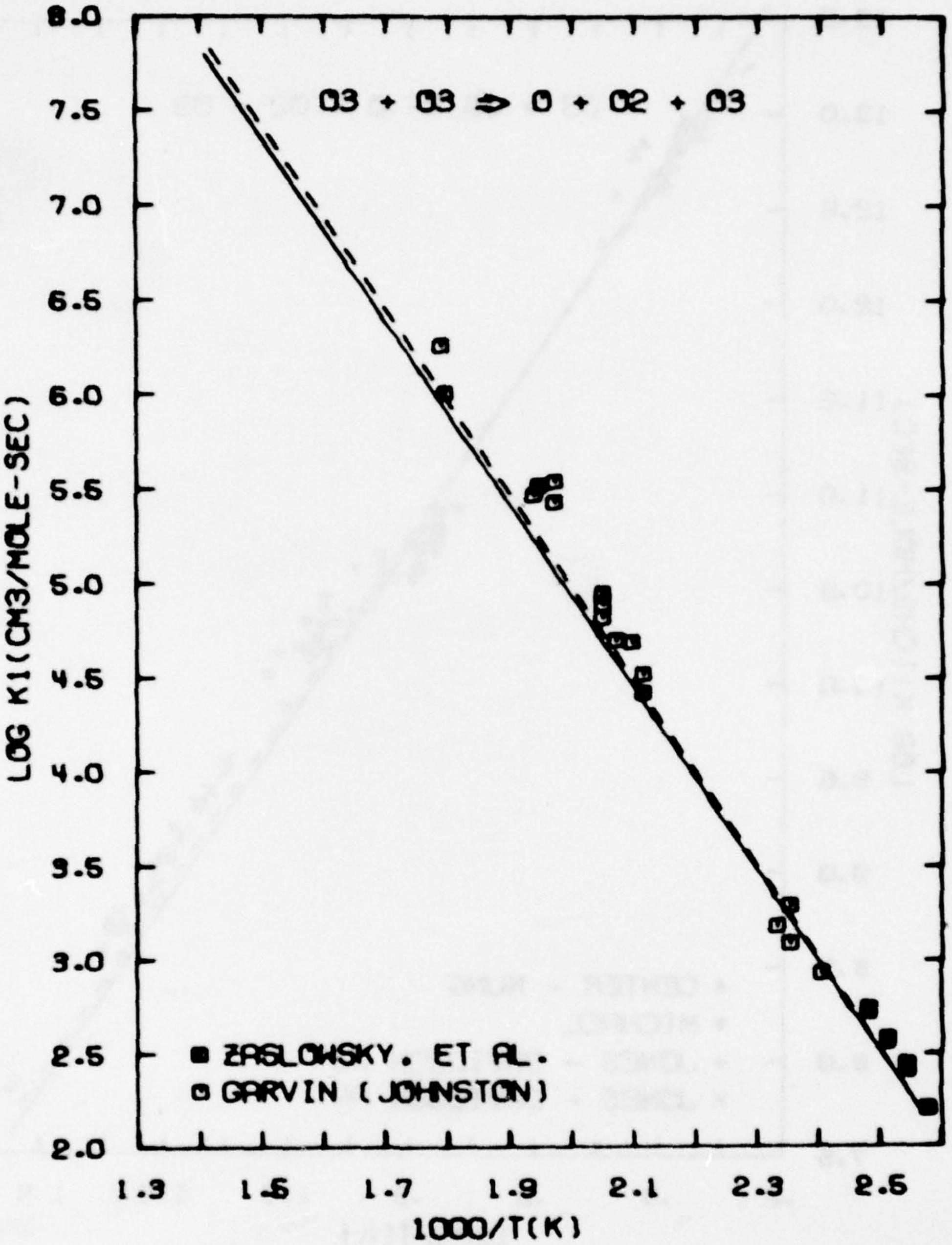

Figure 1b. Intermediate Temperature Range Data for the Unimolecular Ozone Decomposition Reaction. These data are taken from reference 3 of text, Table 18.

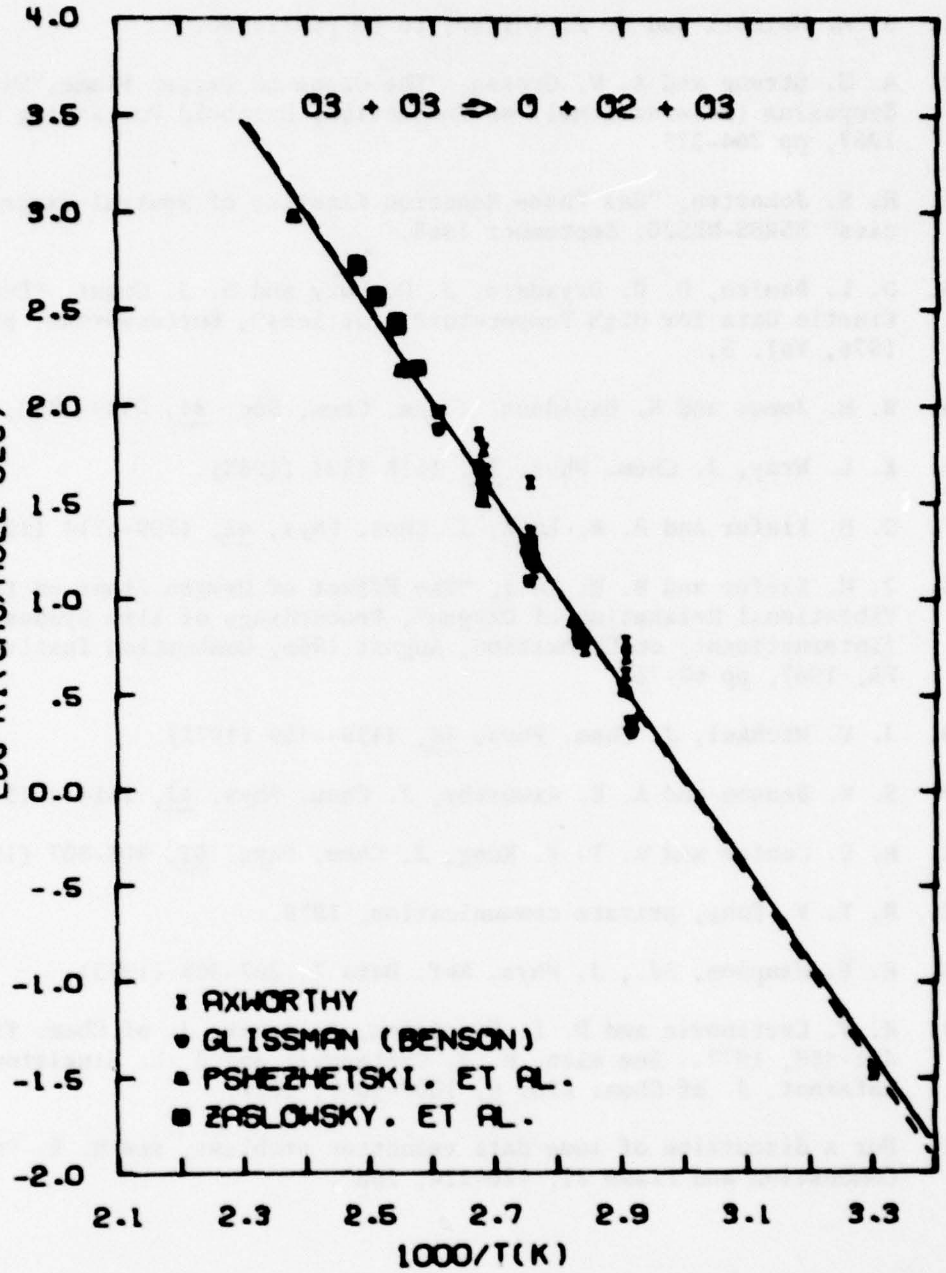

Figure 1c. Low Temperature Range Data for the Unimolecular Ozone Decomposition Reaction. These data are taken from reference 3 of text, Table 18.

REFERENCES

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2. A. G. Streng and A. V. Grosse, "The Ozone to Oxygen Flame,"Sixth Symposium (International) on Combustion, Reinhold Publishing Co., 1957, pp 264-273.

3. H. S. Johnston, "Gas Phase Reaction Kinetics of Neutral Oxygen Species" NSRDS-NBS20, September 1968.

4. D. L. Baulch, D. D. Drysdale, J. Duxbury and S. J. Grant, "Evaluated Kinetic Data for High Temperature Reactions", Butterworths, Boston, 1976, Vol. 3.

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7. J. H. Kiefer and R. W. Lutz, J. Chem. Phys. 42, 1709-1714 (1965).

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9. J. V. Michael, J. Chem. Phys. 54, 4455-4459 (1971).

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11. R. E. Center and R. T. V. Kung, J. Chem. Phys. 62, 801-807 (1975).

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14. R. J. Cvetanovic and D. L. Singleton, Internat. J. of Chem. Kin. 9, 481-488, 1977. See also, R. J. Cvetanovic and D. L. Singleton, Internat. J. of Chem. Kin. 9, 1007-1009, 1977.

15. For a discussion of some data reduction problems, see H. B. Palmer, Combustion and Flame 11, 120-124, 1967.

APPENDIX A. DATA EXCLUSIVE OF CENTER & KUNG

The purpose for this appendix is to list all the data used for this evaluation of k_1 so that, together with Table I, it would be available in one location for future use.

The bulk of Table I-A that comprises this appendix is taken directly from Johnston (reference 3 of text). The only change from his Table 18 is the deletion of the six data points for which Axworthy added H_2O_2 or H_2O to the gaseous mixture. The references for this table are to be found in reference 3 (of text). Following Johnston, these data are listed for equivalent ozone (i.e., $M = O_3$), and we have converted these to cm^3/moles using the conversion 6.023×10^{23} particles/mole.

Michael's data are taken from reference 9 (in text) where equivalent ozone has been found using

$$k_1 \ (M = Ar)/k_1 \ (M = Kr) = 1.25$$

and

$$k_1 \ (M = O_3)/k_1 \ (M = Ar) = 4.0.$$

Table I-A is comprised of three columns. The first lists degrees Kelvin, the second column lists the reciprocal of the first multiplied by 1000. The third column lists the logarithm to the base ten of the rate coefficient for reaction (1) in units of cm^3/mole-sec. All these values are given for ozone as the third body. To convert to other third bodies see references 3 and 9 (of text).

APPENDIX A. DATA EXCLUSIVE OF CENTER & KUNG

The purpose for this appendix is to list all the data used for this evaluation of k_1 so that, together with Table 1, it would be available in one location for future use.

The bulk of Table I-A that comprises this appendix is taken directly from Johnston (reference 1 of text). The only change from his Table [illegible] is the deletion of the six data points for which Kaufman added H_2O_2 or H_2O to the gaseous mixture. The references for this table are to be found in reference 1 (of text). Following Johnston, these data are listed for equivalent [illegible] (M = N_2, M = Ar), and we have converted these to cm^6/molec^2-sec using the conversion 6.023 x 10^{23} particles/mole.

[illegible] data are taken from reference 4 (of text) where equivalent [illegible] has been found using

$$k_1 (M = Ar)/k_1 (M = N_2) = 1.19$$

and

$$k_1 (M = O_2)/k_1 (M = Ar) = 4.0$$

Table I-A is comprised of three columns. The first lists degrees Kelvin, the second column lists the reciprocal of the first multiplied by 1000. The third column lists the logarithm to the base ten of the rate coefficient for reaction (1) in units of cm^6/molec^2-sec. All these values are given for [illegible] as the third body. To convert to other third bodies see references 3 and 4 (of text).

TABLE I-A DATA EXCLUSIVE OF CENTER AND KUNG

JONES AND DAVIDSON DATA (M=AR).

T	1000/T	LOGK1
769.	1.300	8.59
778.	1.285	8.69
779.	1.284	8.73
787.	1.271	8.78
792.	1.263	8.69
812.	1.232	8.85
824.	1.214	8.97
825.	1.212	8.93
827.	1.209	9.02
828.	1.208	9.02
840.	1.190	9.06
840.	1.190	9.11
841.	1.189	9.08
846.	1.182	9.24
871.	1.148	9.37
876.	1.142	9.35
881.	1.135	9.36
890.	1.124	9.63
910.	1.099	9.54
910.	1.099	9.60

JONES AND DAVIDSON DATA (M=N2).

T	1000/T	LOGK1
689.	1.451	7.84
694.	1.441	7.89
788.	1.269	8.74
831.	1.203	9.07
837.	1.195	9.06
855.	1.170	9.18
863.	1.159	9.22

PSHEZHETSKI,ET AL DATA.

T	1000/T	LOGK1
344.	2.907	.52
354.	2.825	.88
373.	2.681	1.51
392.	2.551	2.18
420.	2.381	2.98

ZASLOWSKY,ET AL DATA.

T	1000/T	LOGK1
388.	2.577	2.20
388.	2.577	2.20
393.	2.545	2.42
393.	2.545	2.41
393.	2.545	2.44
393.	2.545	2.41
393.	2.545	2.44
393.	2.545	2.42
393.	2.545	2.43
393.	2.545	2.42

TABLE I-A DATA EXCLUSIVE OF CENTER AND KUNG (Cont'd)

393.	2.545	2.43
398.	2.513	2.56
398.	2.513	2.58
403.	2.481	2.73
403.	2.481	2.74
403.	2.481	2.72

GARVIN DATA.

T	1000/T	LOGK1
416.	2.404	2.93
425.	2.353	3.09
425.	2.353	3.29
429.	2.331	3.18
473.	2.114	4.52
473.	2.114	4.42
477.	2.096	4.69
483.	2.070	4.70
488.	2.049	4.95
488.	2.049	4.89
488.	2.049	4.82
488.	2.049	4.94
507.	1.972	5.54
507.	1.972	5.43
514.	1.946	5.52
516.	1.938	5.47
557.	1.795	6.01
559.	1.789	6.26
559.	1.789	6.28

GLISSMAN DATA.

T	1000/T	LOGK1
343.	2.915	.31
343.	2.915	.37
353.	2.833	.82
353.	2.833	.82
353.	2.833	.82
363.	2.755	1.10
363.	2.755	1.18
363.	2.755	1.20
363.	2.755	1.21
363.	2.755	1.23
363.	2.755	1.23
363.	2.755	1.23
363.	2.755	1.23
363.	2.755	1.24
363.	2.755	1.24
363.	2.755	1.26
363.	2.755	1.26
363.	2.755	1.26
363.	2.755	1.26
363.	2.755	1.27
363.	2.755	1.29
363.	2.755	1.29
363.	2.755	1.30

TABLE I-A. DATA EXCLUSIVE OF CENTER AND KUNG (Cont'd)

363.	2.755	1.31
373.	2.681	1.59
373.	2.681	1.59
373.	2.681	1.63
373.	2.681	1.64
373.	2.681	1.68
383.	2.611	1.89
383.	2.611	1.98
383.	2.611	1.98
353.	2.833	.82
353.	2.833	.82
353.	2.833	.82
363.	2.755	1.23
363.	2.755	1.26
363.	2.755	1.26
363.	2.755	1.26
373.	2.681	1.59
373.	2.681	1.64
373.	2.681	1.64
353.	2.833	.78
353.	2.833	.82
363.	2.755	1.21
363.	2.755	1.23
363.	2.755	1.23
353.	2.833	.78
353.	2.833	.82
363.	2.755	1.23
363.	2.755	1.23
363.	2.755	1.23

AXWORTHY DATA.

T	1000/T	LOGK1
303.	3.300	-1.68
344.	2.907	.78
344.	2.907	.70
344.	2.907	.61
352.	2.841	.76
362.	2.762	1.21
362.	2.762	1.18
363.	2.755	1.30
363.	2.755	1.34
363.	2.755	1.23
363.	2.755	1.26
363.	2.755	1.27
363.	2.755	1.35
363.	2.755	1.61
364.	2.747	1.27
364.	2.747	1.27
364.	2.747	1.29
373.	2.681	1.78
373.	2.681	1.66
374.	2.674	1.69
374.	2.674	1.86

TABLE I-A DATA EXCLUSIVE OF CENTER AND KUNG (Cont'd)

MICHAEL DATA.

T	1000/T	LOGK1
1207.	.829	10.57
1277.	.783	10.75
1255.	.797	10.56
1365.	.763	11.00
1273.	.786	10.63
1285.	.778	10.61
1319.	.758	10.71
1276.	.784	10.68
1384.	.723	10.96
1325.	.755	10.73
1266.	.790	10.79
1326.	.754	10.78
1265.	.791	10.71
1061.	.943	10.31
1146.	.873	10.40
1323.	.756	10.88
1179.	.848	10.50
1119.	.894	10.38
1041.	.961	10.13
1085.	.922	10.33
1334.	.750	10.92
1152.	.868	10.40
1196.	.836	10.61
1323.	.756	10.83
1069.	.935	10.20
1020.	.980	10.70
996.	1.004	9.88
1311.	.763	10.82
1052.	.951	10.18
1260.	.794	10.61
1128.	.887	10.61
1179.	.848	10.69
1033.	.968	10.20
1185.	.844	10.63
1180.	.847	10.57
1158.	.864	10.45
1121.	.892	10.36
1034.	.967	10.33
971.	1.030	10.05
1067.	.937	10.34
1052.	.951	10.25
988.	1.012	10.16
1065.	.939	10.46

APPENDIX B. DATA OF CENTER AND KUNG

The purpose of this appendix is two fold. First and foremost to serve as a repository* for the actual tabular data upon which Center and Kung have published their paper (see Figure 4 of reference 11 in text). The second purpose lies in providing more detail to the analysis given this data.

Center and Kung's data (reference 12) are given in Table B-I. The terms employed are defined in the Glossary for this appendix. In analyzing this data set, the main problem lies in finding a value for k_1 given the measured relaxation time, τ_p.

Provided $k_2[O] << k_1[M]$ in equation 4 (in text) we can write $d[O_3]/dt = -k_1[M][O_3]$. Since their measurements are made after the shock we have

$$[M] = \rho_2 \, [Y_{Ar}/W_{Ar} + 4Y_{O_3}/W_{O_3}], \tag{B-1}$$

where following Johnston (reference 3) we have taken k_1 $(M = O_3) = 4k_1$ $(M = Ar)$. Since 95% or more of the gas is argon it is a good approximation to take $[M]$ = constant. Then equation 7 (in text) can be readily integrated, to wit

$$[O_3] = [O_3]_0 \exp(-k_1[M]t). \tag{B-2}$$

The experiment consists of optically monitoring the ozone concentration and noting the time, τ_p, that the post shock intensity equals the pre-shock intensity. This corresponds to a change in the O_3 concentration equal to ρ_2/ρ_1. Then

$$\ln(\rho_1/\rho_2) = -k_1[M]\,\tau_p. \tag{B-3}$$

We want an expression for k_1 in terms of experimentally measurable parameters. Using equation (B-1), equation (B-3) can be rewritten as

---

**Dr. Kung has graciously consented that this be done since these data do not appear anywhere else.*

$$k_1 = \frac{\ln (\rho_2/\rho_1)}{(\rho_2/\rho_1)\ (\rho_1 \tau_p)\ (Y_{Ar}/W_{Ar} + 4Y_{O_3}/W_{O_3})} \qquad \text{(B-4)}$$

An expression for ρ_1/ρ_1 can be found from the ideal gas law:

$$\rho_1/p_1 = [RT_1\ (Y_{Ar}/W_{Ar} + Y_{O_3}/W_{O_3})]^{-1} \qquad \text{(B-5)}$$

and measuring τ_p in μsec we find

$$k_1\ (M = Ar) = \frac{10^6 \ln (\rho_2/\rho_1)\ RT_1\ (Y_{Ar}/W_{Ar} + Y_{O_3}/W_{O_3})}{(\rho_2/\rho_1)\ (p_1 \tau_p)\ (Y_{Ar}/W_{Ar} + 4\ Y_{O_3}/W_{O_3})}\ \text{cm}^3\ \text{mole}^{-1}\text{s}^{-1}. \qquad \text{(B-6)}$$

Before accepting any value of k_1 derived from equation B-6, we must verify the basic *assumption that* $k_2\ [O] << k_1\ [M]$. To do this, equations (4) and (5) (in text) are integrated numerically. Because of the uncertainty in using expressions for the value of k_2 at the higher temperatures, a value twice as large as the largest recommended value (reference 13 of text) has been used in the numerical integration. Those integrations that gave relaxation times within 10% of the measured relaxation times were accepted as meeting the criterion $k_1\ [M] << k_2\ [O]$.

For example at T_1 = 2041 K, the measured relaxation time is 13.4 μsec. If Hampson's value (reference 13 of text) for k_2 is used, we calculated a 12.7 μsec relaxation time. If twice Hampson's value is used, the relaxation time is found to be 12.2 μsec. Since the term $k_2\ [O]$ in equation 4 (of text) becomes the more important the lower the temperature, the datum at T_1 = 2041 K is the lowest temperature we have accepted.

TABLE B-1. THE DATA COLLECTED BY CENTER AND KUNG

Run	X_{O_3I}	u_s (mm/μs)	p_1 (torr)	ρ_2/ρ_1	$\tau_p p_1$ (atmos-μsec)	$\tau_J p_1$ (atmos-μsec)	1000/T (K^{-1})
686	6	1.27	0.74	3.645	4.5 (-2)*	3.1 (-2)	0.63
687	6	1.53	0.738	3.86	7.7 (-2)	5.6 (-3)	0.47
688	5	1.45	0.725	3.8	1.2 (-3)**	9.0 (-3)	0.515
690	5	1.315	0.70	3.69	3.85(-2)	2.3 (-2)	0.60
691	5	1.30	0.682	3.67	3.9 (-2)	2.5 (-2)	0.61
692	5	1.28	0.675	3.65	4.2 (-2)	2.8 (-2)	0.62
694	5	1.27	0.655	3.645	4.8 (-2)	3.05(-2)	0.63
695	5	1.725	0.650	3.97	4.6 (-3)	1.9 (-3)	0.375
698	5	1.42	0.620	3.77	2.0 (-2)	1.10(-2)	0.53
699	5	1.21	0.610	3.58	0.70	5.3 (-2)	0.67
700	5	1.12	0.603	3.47	0.145	0.135	0.74
701	5	1.06	1.68	3.38	0.255	0.205	0.78
702	5	1.04	2.05	3.35	0.27	0.25	0.80
703	5	1.095	2.41	3.43	0.247	0.145	0.75
710	2	1.59	0.773	3.75	8.2 (-3)	3.5 (-3)	0.40
715	2	0.96	2.72	3.15	0.91	0.74	0.92
716	2	1.01	2.57	3.21	0.61	0.42	0.86
744	5	1.37	0.767	3.73	2.25(-2)	1.52(-2)	0.565
745	5	1.65	0.755	3.93	6.3 (-3)	2.85(-3)	0.41
746	5	1.69	0.425	3.95	6.9 (-3)	2.3 (-3)	0.39
747	5	1.27	0.435	3.65	4.3 (-2)	3.2 (-2)	0.63
748	2	1.42	0.88	3.65	1.55(-2)	1.0 (-2)	0.49
750	2	1.615	0.86	3.77	6.3 (-3)	3.1 (-3)	0.39
751	2	1.14	1.68	3.39	0.14	0.11	0.72
752	2	1.175	1.65	3.43	9.6 (-2)	7.2 (-2)	0.70
753	2	1.27	1.60	3.53	5.1 (-2)	3.1 (-2)	0.60
754	1.3	1.255	3.05	3.4	5.5 (-2)	3.5 (-2)	0.61
757	1.3	0.995	2.82	3.1	0.62	0.57	0.88
758	1.2	0.955	2.75	3.1	0.65	0.57	0.88
759	1.2	1.205	1.38	3.35	7.7 (-2)	5.5 (-2)	0.655
760	1.2	1.235	2.62	3.39	4.2 (-2)	4.2 (-2)	0.625
762	1.2	1.03	2.51	3.15	0.67	0.40	0.835
763	1.2	1.12	2.48	3.25	0.246	0.138	0.755
766	1.0	1.3	2.42	3.44	3.2 (-2)	2.4 (-2)	0.575
767	4.5	1.815	0.4	4.01	3.95(-3)	1.42(-3)	0.34
768	4.5	1.615	0.382	3.91	4.3 (-3)	3.4 (-3)	0.425
769	4.5	1.60	0.378	3.90	4.9 (-3)	3.0 (-3)	0.44
771	4.5	1.715	0.380	3.97	5.5 (-3)	2.12(-3)	0.38
774	4.5	1.77	0.35	3.99	3.35(-3)	1.7 (-3)	0.36
775	4.5	1.743	0.337	3.98	4.1 (-3)	1.87(-3)	0.37
776	4.5	1.79	0.34	4.00	3.35(-3)	1.56(-3)	0.35
782	5	1.41	0.63	3.78	1.6 (-2)	1.2 (-2)	0.54
783	5	1.425	0.613	3.78	1.19(-2)	1.1 (-2)	0.525
784	3/4	0.99	3.02	3.09	0.75	.66	0.89
785	3/4	1.0	2.96	3.1	0.73	.57	0.88
786	3/4	1.0	2.84	3.1	0.69	.57	0.88
787	3/4	1.06	2.75	3.18	0.355	.275	0.80
789	3/4	1.05	2.60	3.17	0.43	.31	0.81
790	3/4	0.97	2.55	3.06	0.97	.85	0.91
791	3/4	1.035	2.47	3.15	0.43	.37	0.83
788	3/4	1.03	2.68	3.15	0.46	.4	0.835

* *Read 4.5(-2) as 4.5×10^{-2}*

***Apparent misprint, we take this value to be 1.2(-2)*

GLOSSARY FOR APPENDIX B

$X_{O_3 I}$ Initial mole fraction of O_3.

u_s Shock speed (mm μsec^{-1}).

p_1 Initial pressure (torr).

ρ_1 Initial density (gm/cm^3).

ρ_2 Post-shock density (gm/cm^3).

t_p Relaxation time measured by Center and Kung (μsec). This is the time in which the O_3 concentration changes by a factor of ρ_2/ρ_1.

τ_J Relaxation time predicted by Johnston recommended rates (μsec).

$\tau_\rho p_1$ Relaxation time multiplied by initial pressure (μsec - atm).

T_1 Initial temperature (K).

Y_{Ar} Mass fraction of argon.

Y_{O_3} Mass fraction of ozone.

W_{Ar} Molecular weight of argon (40 gm/mole).

W_{O_3} Molecular weight of ozone (48 gm/mole).

R Gas constant (82.05 cm^3 - atm/mole-deg).

[M] Concentration of "third" body, (moles/cm^3).

APPENDIX C. LEAST SQUARES FITTING PROGRAM

Below is a listing of the subroutine used to compute a least square fit to k_1 using the data listed in Appendix A and Table I. The program can be easily modified to produce three parameter fits of the form $aT^b \exp(C/T)$.

```
      PROGRAM RTK1(OUTPUT,TAPE6=OUTPUT)
      COMMON/TAHLS/A,B,C
      DIMENSION T(218),RK1(218),LGK1(218)
      DIMENSION TK(218)
      DIMENSION TT(218)
      DIMENSION RK2(6)
      REAL LGK1
C  DATA FOR THE RATE CONSTANT OF THE EQUATION
C  O3 + M = O2 + O + M
C  THE RATE CONSTNATS ARE IN THE UNITS  CM**3/PARTICLE-SECOND
C  THE DATA IS THEN THE NEGATIVE OF THE LOG OF THE RATE CONSTANTS
C  ALL DATA IS GIVEN IN TERMS OF M = O3
C  JONES AND DAVIDSON DATA    M = ARGON   20 POINTS
      DATA (T   (L),L=1  ,20 ) /
     * 769.,778.,779.,787.,792.,
     * 812.,824.,825.,827.,828.,
     * 840.,840.,841.,846.,871.,
     * 876.,881.,890.,910.,910. /
      DATA (LGK1(L),L=1  ,20 ) /
     * 15.19 ,15.09 ,15.05 ,15.00 ,15.09 ,
     * 14.93 ,14.81 ,14.85 ,14.76 ,14.76 ,
     * 14.72 ,14.67 ,14.70 ,14.54 ,14.61 ,
     * 14.63 ,14.44 ,14.35 ,14.24 ,14.18 /
C  JONES AND DAVIDSON DATA    M = N2    7 POINTS
      DATA (T   (L),L=21 ,27 ) /
     * 689.,694.,788.,831.,837.,855.,863. /
      DATA (LGK1(L),L=21 ,27 ) /
     * 15.94 ,15.89 ,15.04 ,14.71 ,14.72 ,14.60 ,14.56 /
C  PSHEZHETSKI DATA    M = O3    5 POINTS
      DATA (T   (L),L=28 ,32 ) /
     * 344.,354.,373.,392.,420. /
      DATA (LGK1(L),L=28 ,32 ) /
     * 23.26 ,22.90 ,22.27 ,21.60 ,20.80 /
C  ZASLONSKY DATA    M = O3   16 POINTS
      DATA (T   (L),L=33 ,48 ) /
     * 388.,388.,393.,393.,393.,393.,393.,393.,
     * 393.,393.,393.,398.,398.,403.,403.,403. /
      DATA (LGK1(L),L=33 ,48 ) /
     * 21.58 ,21.56 ,21.36 ,21.37 ,21.34 ,21.37 ,21.34 ,21.36 ,
     * 21.35 ,21.36 ,21.35 ,21.22 ,21.20 ,21.05 ,21.04 ,21.06 /
C  GARVIN DATA   MASSAGED BY JOHNSTON    M = O3      19 POINTS
      DATA (T   (L),L=49 ,67 ) /
     * 416.,425.,425.,429.,473.,473.,477.,
     * 483.,488.,488.,488.,488.,
     * 507.,507.,514.,516.,557.,559.,559. /
      DATA (LGK1(L),L=49 ,67 ) /
     * 20.85 ,20.69 ,20.69 ,20.60 ,19.26 ,19.36 ,19.09 ,
     * 19.08 ,18.83 ,18.49 ,18.46 ,18.84 ,
     * 18.24 ,18.35 ,18.26 ,18.31 ,17.77 ,17.52 ,17.52 /
C  GLISSMAN DATA   MASSAGED BY HENSON   M = O3   52 POINTS
      DATA (T   (L),L=68 ,119) /
     * 343.,343.,353.,353.,353.,363.,363.,363.,
     * 363.,363.,363.,363.,363.,
     * 363.,363.,363.,363.,363.,
     * 363.,363.,363.,363.,363.,
     * 363.,373.,373.,373.,373.,
     * 373.,383.,383.,383.,353.,
```

```
     * 353. .353. .363. .363. .363. .
     * 363. .373. .373. .373. .353. .
     * 353. .363. .363. .363. .353. .353. .363. .363. .363. /
      DATA (LGK1(L),L=68 ,119) /
     * 23.67 .23.41 .22.96 .22.96 .22.96 .22.68 .22.68 .22.58 .
     * 22.57 .22.55 .22.55 .22.55 .22.55 .
     * 22.56 .22.56 .22.52 .22.52 .22.52 .
     * 22.52 .22.51 .22.49 .22.49 .22.48 .
     * 22.47 .22.19 .22.19 .22.15 .22.14 .
     * 22.10 .21.80 .21.80 .21.80 .22.96 .
     * 22.96 .22.96 .22.55 .22.56 .22.54 .
     * 22.52 .22.19 .22.14 .22.14 .23.00 .
     * 22.96 .22.57 .22.55 .22.55 .23.00 .
     * 22.96 .22.55 .22.55 .22.55 /
C  ARWORTHY DATA    M = 03      21 POINTS
      DATA (T    (L),L=120,140) /
     * 303. .344. .344. .344. .352. .362. .
     * 362. .363. .363. .363. .363. .363. .363. .363. .
     * 364. .364. .364. .373. .373. .376. .376. /
      DATA (LGK1(L),L=120,140) /
     * 25.26 .23.80 .23.08 .23.17 .23.04 .22.57 .
     * 22.60 .22.48 .22.44 .22.55 .22.52 .22.51 .22.43 .22.17 .
     * 22.51 .22.51 .22.49 .22.00 .22.14 .22.09 .21.92 /
C  MICHAEL DATA    M = KRYTON    43 POINTS
C K(M=KR)(LITER*E-7/MOLE-S) = 8.30E-14*K(M=O3)(CM**3/PARTICLE-S)
      DATA (T    (L),L=141,183) /
     * 1207. .1277. .1255. .1365. .1273. .1285. .1319. .1276. .1384. .
     * 1325. .1266. .1326. .1265. .1061. .1144. .1323. .1179. .
     * 1119. .1061. .1085. .1334. .1152. .1196. .
     * 1323. .1069. .1020. .996. .1311. .1052. .1260. .
     * 1178. .1179. .1033. .1185. .1188. .1158. .1121. .
     * 1034. .971. .1067. .1052. .988. .1065. /
      DATA (LGK1(L),L=141,183) /
     * 13.21 .13.03 .13.22 .12.78 .13.15 .13.17 .13.07 .13.10 .12.84 .
     * 13.05 .12.99 .13.00 .13.07 .13.47 .13.38 .12.90 .
     * 13.28 .13.40 .13.65 .13.45 .12.86 .13.34 .13.17 .
     * 12.95 .13.58 .13.58 .13.90 .12.96 .13.60 .13.17 .
     * 13.17 .13.09 .13.58 .13.15 .13.21 .13.33 .13.42 .
     * 13.45 .13.73 .13.39 .13.53 .13.62 .13.32 /
C  CENTER AND KUNG DATA FROM TABLE.
C  USING FORMULA I DERIVED.
C  THIS DATA IS IN UNITS CM**3/MOLE-SECOND. M=ARGON.
      DATA (T(L),L=184,197) /
     * 2041. .2128. .2273. .2353. .2439. .2500. .2564. .
     * 2564. .2632. .2667. .2703. .2778. .2857. .2941. /
      DATA (RK1(L),L=184,197) /
     * 5.31E11.9.48E11.1.56E12.1.76E12.1.18E12.9.98E11.1.08E12.
     * 1.30E12.1.37E12.1.62E12.1.84E12.2.25E12.2.24E12.1.90E12 /
      DO 10 K=1,183
      LGK1(K)=-LGK1(K)
      RK1(K)=10**LGK1(K)
C  CONVERT TO CM**3/MOLE-SECOND.
      RK1(K)=RK1(K)*6.023E23
 10   CONTINUE
C  CONVERT CENTER AND KUNG DATA TO M = O3
      DO 15 K=184,197
 15   RK1(K)=RK1(K)*4.
```

```
      M=197
      WRITE(6,25)M
 25   FORMAT(/5X,20HNO. OF DATA POINTS =,I8)
      CALL SOLST(T,RK1,M)
      STOP
      END
```

```
      SUBROUTINE SQLST(X,Y,M)
      DIMENSION X(218),Y(218),W(218),WR(218),
     * AL(218),XV(218),YL(218),YP(218)
      DIMENSION RS(2),SL(2)
      COMMON/TAMA/UL(2,2)
C  **************************
C  REFERENCES.
C  R.J. CVETANOVIC AND D.L. SINGLETON.
C  INTERNAT. J. OF CHEM. KIN. 9.
C  PP. 481-488. 1007-1009. 1977.
C  **************************
C  ERRORS ARE MEASURED IN A RELATIVE SENSE.
      DO 15 K=1,M
15    WR(K)=1.0/(Y(K)*Y(K))
C  EACH GROUP OF DATA IS WEIGHTED EQUALLY.
      DO 16 K=1,27
16    WR(K)=WR(K)/27.
      DO 17 K=28,140
17    WR(K)=WR(K)/113.
      DO 18 K=141,183
18    WR(K)=WR(K)/43.
      DO 19 K=184,197
19    WR(K)=WR(K)/14.
C  LEAST SQUARES FIT BY A FUNCTION OF THE FORM
C  Y = A * EXP( C/X )                                              EXP
C  **************************
C  A FIT BY A FUNCTION OF THE FORM
C  Y = A * (X**B)
C  CAN BE MADE BY CHANGING THE CARDS WITH EXP AT THE RIGHT.
C  XV(K)=1./X(K) MUST BE REPLACED BY XL(K)=ALOG(X(K))
C  **************************
      A=0.0
      C=0.0                                                        EXP
C  WE WILL ACTUALLY WORK WITH A FIT OF THE FORM
C  LN Y = LN A + C/X
C  THE WEIGHTS MUST BE TRANSFORMED.
C  THIS IS A FIRST APPROXIMATION TO THE CORRECT TRANSFORMED WEIGHTS.
      DO 20 K=1,M
      W(K)=Y(K)*Y(K)*WR(K)
      XV(K)=1./X(K)                                                EXP
20    YL(K)=ALOG(Y(K))
C  ITERATE TO FIND THE CORRECT TRANSFORMED WEIGHTS.
      DO 500 NCT=1,10
      DO 30 I=1,2
      RS(I)=0.0
      DO 30 J=1,2
30    UL(I,J)=0.0
      DO 40 K=1,M
      UL(1,1)=UL(1,1)+W(K)
      UL(2,1)=UL(2,1)+XV(K)*W(K)                                   EXP
      UL(2,2)=UL(2,2)+XV(K)*XV(K)*W(K)                             EXP
      RS(1)=RS(1)+YL(K)*W(K)
      RS(2)=RS(2)+YL(K)*XV(K)*W(K)                                 EXP
40    CONTINUE
      UL(1,2)=UL(2,1)
C  SOLVE FOR A AND C BY SOLVING THE APPROPRIATE SET OF TWO
C  EQUATIONS IN TWO UNKNOWNS.
```

```
      CALL DECOMP(2)
      CALL SOLVE(2,WS,SL)
      AN=EXP(SL(1))                                              EXP
      CN=SL(2)                                                   EXP
      WRITE(6,130)AN,CN                                          EXP
130   FORMAT(2X,3HA =,1PE12.4,10X,3HC =,1PE12.4)
C  COMPARE THE VALUES FROM THE FIT WITH THE ORIGINAL DATA AND GET A
C  WEIGHTED ERROR TERM.
      DO 50 K=1,M                                                EXP
50    YP(K)=AN*EXP(CN/X(K))
      ERR=0.0
      DO 60 K=1,M
      D=Y(K)-YP(K)
      PC=ABS(D/Y(K))
      ERR=ERR+W(K)*(D**2)
60    CONTINUE
      ERR=SQRT(ERR/FLOAT(M))
      WRITE(6,140)ERR
140   FORMAT(2X,16HWEIGHTED ERROR =,1PE12.4)
C  COMPARE THE NEW VALUES OF A AND C WITH THE VALUES FROM THE PREVIOUS
C  ITERATION.  IF THEY ARE CLOSE ENOUGH, END THE ITERATION.
      D1=ABS(AN-A)/ABS(AN)                                       EXP
      D2=ABS(CN-C)/ABS(CN)
      IF(D1.LT.1.0E-5.AND.D2.LT.1.0E-5)GO TO 1000
C  OTHERWISE,REDEFINE THE TRANSFORMED WEIGHTS AND ITERATE AGAIN.
      A=AN                                                       EXP
      C=CN
      DO 70 K=1,M
70    W(K)=YP(K)*(Y(K)-YP(K))*WR(K)/ALOG(Y(K)/YP(K))
500   CONTINUE
1000  CONTINUE
C  FIND THE RELATIVE ERROR.
      ERR=0.0
      DO 1050 K=1,M
      D=Y(K)-YP(K)
      PC=ABS(D/Y(K))
      ERR=ERR+PC**2
      WRITE(6,120)X(K),Y(K),YP(K),D,PC
1050  CONTINUE
      ERR=SQRT(ERR/FLOAT(M))
      WRITE(6,1070)ERR
1070  FORMAT(2X,11HREL ERROR =,1PE12.4)
120   FORMAT(1P5E12.4)
      RETURN
      END
```

```
      SUBROUTINE DECOMP(NN)
      DIMENSION SCALES( 2)
      COMMON/DS/IPS( 2)
      COMMON/TAMB/UL(2,2)
C  THIS IS A STANDARD ALGORITHM FOR SOLVING A SET OF LINEAR
C  ALGEBRAIC EQUATIONS USING AN LU DECOMPOSITION AND
C  BACK SUBSTITUTION.
C  REFERENCE.
C  FORSYTHE AND MOLER.  COMPUTER SOLUTION OF LINEAR ALGEBRAIC SYSTEMS.
      N=NN
      DO 5 I=1,N
      IPS(I)=I
      ROWNRM=0.0
      DO 2 J=1,N
      IF(ROWNRM-ABS(UL(I,J)))1,2,2
    1 ROWNRM=ABS(UL(I,J))
    2 CONTINUE
      IF(ROWNRM)3,4,3
    3 SCALES(I)=1.0/ROWNRM
      GO TO 5
    4 CALL SING(1)
      SCALES(I)=0.0
    5 CONTINUE
      NM1=N-1
      DO 17 K=1,NM1
      BIG=0.0
      DO 11 I=K,N
      IP=IPS(I)
      SIZE=ABS(UL(IP,K))*SCALES(IP)
      IF(SIZE-BIG)11,11,10
   10 BIG=SIZE
      IDXPIV=I
   11 CONTINUE
      IF(BIG)13,12,13
   12 CALL SING(2)
      GO TO 17
   13 IF(IDXPIV-K)14,15,14
   14 J=IPS(K)
      IPS(K)=IPS(IDXPIV)
      IPS(IDXPIV)=J
   15 KP=IPS(K)
      PIVOT=UL(KP,K)
      KP1=K+1
      DO 16 I=KP1,N
      IP=IPS(I)
      EM=-UL(IP,K)/PIVOT
      UL(IP,K)=-EM
      DO 16 J=KP1,N
      UL(IP,J)=UL(IP,J)+EM*UL(KP,J)
   16 CONTINUE
   17 CONTINUE
      KP=IPS(N)
      IF(UL(KP,N))19,18,19
   18 CALL SING(2)
   19 RETURN
      END
```

```
      SUBROUTINE SOLVE(NN,B,X)
      DIMENSION B( 2),X( 2)
      COMMON/DS/IPS( 2)
      COMMON/TAB6/UL(2,2)
      N=NN
      NP1=N+1
      IP=IPS(1)
      X(1)=B(IP)
      DO 2 I=2,N
      IP=IPS(I)
      IM1=I-1
      SUM=0.0
      DO 1 J=1,IM1
    1 SUM=SUM+UL(IP,J)*X(J)
    2 X(I)=B(IP)-SUM
      IP=IPS(N)
      X(N)=X(N)/UL(IP,N)
      DO 4 IBACK=2,N
      I=NP1-IBACK
      IP=IPS(I)
      IP1=I +1
      SUM=0.0
      DO 3 J=IP1,N
    3 SUM=SUM+UL(IP,J)*X(J)
    4 X(I)=(X(I)-SUM)/UL(IP,I)
      RETURN
      END
```

```
      SUBROUTINE SING(IWHY)
      NOUT=6
      IF(IWHY.EQ.1)WRITE(NOUT,11)
      IF(IWHY.EQ.2)WRITE(NOUT,12)
11    FORMAT(54H0MATRIX WITH ZERO ROW IN DECOMPOSE.                   )
12    FORMAT(54H0SINGULAR MATRIX IN DECOMPOSE.  ZERO DIVIDE IN SOLVE. )
      RETURN
      END
```

```
          S C O P E   2   L O A D   M A P                                   LOADER VERSION 1.0    11/30/78  13.38.44.  PAGE   1

PROGRAM  WILL BE ENTERED AT  RTKI        (   137)                          SCM LENGTH     11426          LCM LENGTH          0

          BLOCK          ADDRESS     LENGTH       FILE

           /TABLS/          110          3        LGO
          RTKI              113       2200        LGO
           /TAB6/          2313          4        LGO
          SOLST            2317       3040        LGO
           /DS/            5357          2        LGO
          DECOMP           5361        164        LGO
          SOLVE            5545        127        LGO
          SING             5674         44        LGO
            /STP.END/      5740          1     SL-FTNLIB
            /FCL.C./       5741         23     SL-FTNLIB
            /QB.IO./       5764        136     SL-FTNLIB
          QBNTRY=          6122          1     SL-FTNLIB
          COMIO=           6123         44     SL-FTNLIB
          FECMSK=          6167         41     SL-FTNLIB
          FLTOUT=          6230        315     SL-FTNLIB
          FMTAP=           6545        373     SL-FTNLIB
          FORSYS=          7140        533     SL-FTNLIB
          FORUTL=          7673         44     SL-FTNLIB
          GETFIT=          7737         43     SL-FTNLIB
          KODER=          10002        467     SL-FTNLIB
          OUTC=           10471        171     SL-FTNLIB
          OUTCOM=         10662        204     SL-FTNLIB
          ALOG            11066         77     SL-FTNLIB
          EXP             11165        100     SL-FTNLIB
          ITOX=           11265         10     SL-FTNLIB
          SQRT            11275         46     SL-FTNLIB
          SYSAID=         11343          1     SL-FTNLIB
          SYS=1ST         11344         62     SL-FTNLIB

   NO. OF DATA POINTS =      197
A =  5.6896E+14           C = -1.1195E+04
WEIGHTED ERROR =  5.7654E-02
A =  4.2780E+14               C = -1.1156E+04
WEIGHTED ERROR =  4.9489E-02
A =  4.3174E+14               C = -1.1161E+04
WEIGHTED ERROR =  4.9484E-02
A =  4.3131E+14               C = -1.1161E+04
WEIGHTED ERROR =  4.9484E-02
A =  4.3137E+14               C = -1.1161E+04
WEIGHTED ERROR =  4.9484E-02
A =  4.3136E+14               C = -1.1161E+04
WEIGHTED ERROR =  4.9484E-02
A =  4.3136E+14               C = -1.1161E+04
WEIGHTED ERROR =  4.9484E-02
7.6900E+02  3.8888E+08  2.1467E+08  1.7421E+08  4.4797E-01
7.7800E+02  4.8957E+08  2.5392E+08  2.3565E+08  4.8135E-01
7.7900E+02  5.3680E+08  2.5863E+08  2.7817E+08  5.1819E-01
7.8700E+02  6.0230E+08  2.9918E+08  3.0312E+08  5.0327E-01
7.9200E+02  4.8957E+08  3.2720E+08  1.5236E+08  3.3165E-01
8.1200E+02  7.0764E+08  4.6298E+08  2.4467E+08  3.4575E-01
8.2400E+02  9.3285E+08  5.6557E+08  3.6728E+08  3.9372E-01
8.2500E+02  8.5077E+08  5.7494E+08  2.7584E+08  3.2422E-01
8.2700E+02  1.0467E+09  5.9406E+08  4.5262E+08  4.3244E-01
8.2800E+02  1.0467E+09  6.0382E+08  4.4286E+08  4.2311E-01
8.4000E+02  1.1477E+09  7.3204E+08  4.1562E+08  3.6215E-01
```

8.6000E+02	1.2877E+09	7.3204E+08	5.5566E+08	4.3151E-01
8.6100E+02	1.2017E+09	7.6370E+08	4.5805E+08	3.8115E-01
8.6600E+02	1.7371E+09	8.0437E+08	9.3264E+08	5.3693E-01
8.7100E+02	2.3432E+09	1.1766E+09	1.1666E+09	4.9870E-01
8.7600E+02	2.2378E+09	1.2638E+09	9.7398E+08	4.3525E-01
8.8100E+02	2.1868E+09	1.3585E+09	8.2828E+08	3.7876E-01
8.9000E+02	2.6904E+09	1.5442E+09	1.1462E+09	4.2602E-01
9.1000E+02	3.4659E+09	2.0342E+09	1.4316E+09	4.1306E-01
9.1000E+02	3.9794E+09	2.0342E+09	1.9451E+09	4.8880E-01
6.8900E+02	6.9153E+07	3.9804E+07	2.9350E+07	4.2441E-01
6.9400E+02	7.7591E+07	4.6731E+07	3.2860E+07	4.2351E-01
7.8800E+02	5.4930E+08	3.0462E+08	2.4469E+08	4.4545E-01
8.3100E+02	1.1764E+09	6.3393E+08	5.4046E+08	4.6021E-01
8.3700E+02	1.1477E+09	6.9799E+08	4.4967E+08	3.9181E-01
8.5500E+02	1.5129E+09	9.2420E+08	5.8871E+08	3.8912E-01
8.6300E+02	1.6589E+09	1.0431E+09	6.1579E+08	3.7121E-01
3.4600E+02	3.3099E+00	3.5039E+00	-1.9403E-01	5.8621E-02
3.5400E+02	7.5825E+00	8.7616E+00	-1.1791E+00	1.5550E-01
3.7300E+02	3.2345E+01	4.3656E+01	-1.1311E+01	3.4968E-01
3.9200E+02	1.5129E+02	1.8616E+02	-3.4873E+01	2.3050E-01
4.2000E+02	9.5458E+02	1.2423E+03	-2.8771E+02	3.0140E-01
3.8800E+02	1.5842E+02	1.3881E+02	1.9611E+01	1.2379E-01
3.8800E+02	1.5842E+02	1.3881E+02	1.9611E+01	1.2379E-01
3.9300E+02	2.6291E+02	2.0015E+02	6.2762E+01	2.3872E-01
3.9300E+02	2.5693E+02	2.0015E+02	5.6778E+01	2.2099E-01
3.9300E+02	2.7530E+02	2.0015E+02	7.5153E+01	2.7298E-01
3.9300E+02	2.5693E+02	2.0015E+02	5.6778E+01	2.2099E-01
3.9300E+02	2.7530E+02	2.0015E+02	7.5153E+01	2.7298E-01
3.9300E+02	2.6291E+02	2.0015E+02	6.2762E+01	2.3872E-01
3.9300E+02	2.6904E+02	2.0015E+02	6.8886E+01	2.5605E-01
3.9300E+02	2.6291E+02	2.0015E+02	6.2762E+01	2.3872E-01
3.9300E+02	2.6904E+02	2.0015E+02	6.8886E+01	2.5605E-01
3.9800E+02	3.6292E+02	2.8596E+02	7.6964E+01	2.1207E-01
3.9800E+02	3.8003E+02	2.8596E+02	9.4068E+01	2.4753E-01
4.0300E+02	5.3680E+02	4.0495E+02	1.3185E+02	2.4563E-01
4.0300E+02	5.4930E+02	4.0495E+02	1.4436E+02	2.6280E-01
4.0300E+02	5.2458E+02	4.0495E+02	1.1963E+02	2.2805E-01
4.1400E+02	8.5077E+02	9.6218E+02	-1.1141E+02	1.3095E-01
4.2500E+02	1.2297E+03	1.6982E+03	-4.6849E+02	3.8097E-01
4.2500E+02	1.9490E+03	1.6982E+03	2.5077E+02	1.2867E-01
4.2900E+02	1.5129E+03	2.1694E+03	-6.5647E+02	4.3391E-01
4.7300E+02	3.3099E+04	2.4398E+04	8.7005E+03	2.6287E-01
4.7300E+02	2.6291E+04	2.4398E+04	1.8930E+03	7.2003E-02
4.7700E+02	4.8957E+04	2.9737E+04	1.9220E+04	3.9259E-01
4.8300E+02	5.0097E+04	3.9767E+04	1.0330E+04	2.0620E-01
4.8800E+02	8.9087E+04	5.0390E+04	3.8697E+04	4.3437E-01
4.8800E+02	7.7591E+04	5.0390E+04	2.7201E+04	3.5057E-01
4.8800E+02	6.6041E+04	5.0390E+04	1.5651E+04	2.3699E-01
4.8800E+02	8.7059E+04	5.0390E+04	3.6669E+04	4.2120E-01
5.0700E+02	3.4659E+05	1.1873E+05	2.2786E+05	6.5743E-01
5.0700E+02	2.6904E+05	1.1873E+05	1.5031E+05	5.5868E-01
5.1400E+02	3.3099E+05	1.6024E+05	1.7075E+05	5.1588E-01
5.1600E+02	2.9499E+05	1.7431E+05	1.2069E+05	4.0911E-01
5.5700E+02	1.0229E+06	8.5657E+05	1.6629E+05	1.6257E-01
5.5900E+02	1.8189E+06	9.2023E+05	8.9869E+05	4.9408E-01
5.5900E+02	1.8189E+06	9.2023E+05	8.9869E+05	4.9408E-01
3.4300E+02	2.0409E+00	3.1877E+00	-1.1468E+00	5.6193E-01
3.4300E+02	2.3432E+00	3.1877E+00	-8.4446E-01	3.6038E-01
3.5300E+02	6.6041E+00	8.0130E+00	-1.4089E+00	2.1334E-01
3.5300E+02	6.6041E+00	8.0130E+00	-1.4089E+00	2.1334E-01
3.5300E+02	6.6041E+00	8.0130E+00	-1.4089E+00	2.1334E-01
3.6300E+02	1.2584E+01	1.9145E+01	-6.5615E+00	5.2142E-01
3.6300E+02	1.2584E+01	1.9145E+01	-6.5615E+00	5.2142E-01

3.6300E+02	1.5842E+01	1.9165E+01	-3.3032E+00	2.0851E-01
3.6300E+02	1.6211E+01	1.9165E+01	-2.9362E+00	1.8100E-01
3.6300E+02	1.6975E+01	1.9165E+01	-2.1702E+00	1.2784E-01
3.6300E+02	1.6975E+01	1.9165E+01	-2.1702E+00	1.2784E-01
3.6300E+02	1.6975E+01	1.9165E+01	-2.1702E+00	1.2784E-01
3.6300E+02	1.6975E+01	1.9165E+01	-2.1702E+00	1.2784E-01
3.6300E+02	1.7371E+01	1.9165E+01	-1.7768E+00	1.0217E-01
3.6300E+02	1.7371E+01	1.9165E+01	-1.7768E+00	1.0217E-01
3.6300E+02	1.8189E+01	1.9165E+01	-9.5611E-01	5.2565E-02
3.6300E+02	1.8189E+01	1.9165E+01	-9.5611E-01	5.2565E-02
3.6300E+02	1.8189E+01	1.9165E+01	-9.5611E-01	5.2565E-02
3.6300E+02	1.8189E+01	1.9165E+01	-9.5611E-01	5.2565E-02
3.6300E+02	1.8613E+01	1.9165E+01	-5.3243E-01	2.8608E-02
3.6300E+02	1.9490E+01	1.9165E+01	3.4476E-01	1.7689E-02
3.6300E+02	1.9490E+01	1.9165E+01	3.4476E-01	1.7689E-02
3.6300E+02	1.9944E+01	1.9165E+01	7.9875E-01	4.0049E-02
3.6300E+02	2.0409E+01	1.9165E+01	1.2633E+00	6.1901E-02
3.7300E+02	3.8888E+01	4.3656E+01	-4.7684E+00	1.2262E-01
3.7300E+02	3.8888E+01	4.3656E+01	-4.7684E+00	1.2262E-01
3.7300E+02	4.2640E+01	4.3656E+01	-1.0165E+00	2.3840E-02
3.7300E+02	4.3633E+01	4.3656E+01	-2.3346E-02	5.3501E-04
3.7300E+02	4.7842E+01	4.3656E+01	4.1863E+00	8.7501E-02
3.8300E+02	7.7591E+01	9.5353E+01	-1.7762E+01	2.2892E-01
3.8300E+02	9.5458E+01	9.5353E+01	1.0500E-01	1.0999E-03
3.8300E+02	9.5458E+01	9.5353E+01	1.0500E-01	1.0999E-03
3.5300E+02	6.6041E+00	8.0130E+00	-1.4089E+00	2.1334E-01
3.5300E+02	6.6041E+00	8.0130E+00	-1.4089E+00	2.1334E-01
3.5300E+02	6.6041E+00	8.0130E+00	-1.4089E+00	2.1334E-01
3.6300E+02	1.6975E+01	1.9165E+01	-2.1702E+00	1.2784E-01
3.6300E+02	1.7371E+01	1.9165E+01	-1.7764E+00	1.0217E-01
3.6300E+02	1.7371E+01	1.9165E+01	-1.7768E+00	1.0217E-01
3.6300E+02	1.8189E+01	1.9165E+01	-9.5611E-01	5.2565E-02
3.7300E+02	3.8888E+01	4.3656E+01	-4.7684E+00	1.2262E-01
3.7300E+02	4.3633E+01	4.3656E+01	-2.3346E-02	5.3501E-04
3.7300E+02	4.3633E+01	4.3656E+01	-2.3346E-02	5.3501E-04
3.5300E+02	6.0230E+00	8.0130E+00	-1.9900E+00	3.3040E-01
3.5300E+02	6.6041E+00	8.0130E+00	-1.4089E+00	2.1334E-01
3.6300E+02	1.6211E+01	1.9165E+01	-2.9362E+00	1.8100E-01
3.6300E+02	1.6975E+01	1.9165E+01	-2.1702E+00	1.2784E-01
3.6300E+02	1.6975E+01	1.9165E+01	-2.1702E+00	1.2784E-01
3.5300E+02	6.0230E+00	8.0130E+00	-1.9900E+00	3.3040E-01
3.5300E+02	6.6041E+00	8.0130E+00	-1.4089E+00	2.1334E-01
3.6300E+02	1.6975E+01	1.9165E+01	-2.1702E+00	1.2784E-01
3.6300E+02	1.6975E+01	1.9165E+01	-2.1702E+00	1.2784E-01
3.6300E+02	1.6975E+01	1.9165E+01	-2.1702E+00	1.2784E-01
3.0300E+02	3.3099E-02	4.3446E-02	-1.0347E-02	3.1260E-01
3.4400E+02	6.0230E+00	3.5039E+00	2.5191E+00	4.1824E-01
3.4400E+02	5.0097E+00	3.5039E+00	1.5058E+00	3.0058E-01
3.4400E+02	4.0720E+00	3.5039E+00	5.6813E-01	1.3952E-01
3.5200E+02	5.4930E+00	7.3247E+00	-1.8316E+00	3.3344E-01
3.6200E+02	1.6211E+01	1.7586E+01	-1.3752E+00	8.4833E-02
3.6200E+02	1.5129E+01	1.7586E+01	-2.4573E+00	1.6242E-01
3.6300E+02	1.9944E+01	1.9165E+01	7.9875E-01	4.0049E-02
3.6300E+02	2.1888E+01	1.9165E+01	2.7229E+00	1.2451E-01
3.6300E+02	1.6975E+01	1.9165E+01	-2.1702E+00	1.2784E-01
3.6300E+02	1.8189E+01	1.9165E+01	-9.5611E-01	5.2565E-02
3.6300E+02	1.8613E+01	1.9165E+01	-5.3243E-01	2.8608E-02
3.6300E+02	2.2388E+01	1.9165E+01	3.2232E+00	1.4444E-01
3.6300E+02	4.0720E+01	1.9165E+01	2.1575E+01	5.2984E-01
3.6400E+02	1.8613E+01	2.0833E+01	-2.2198E+00	1.1926E-01
3.6400E+02	1.8613E+01	2.0833E+01	-2.2194E+00	1.1926E-01
3.6400E+02	1.9490E+01	2.0833E+01	-1.3426E+00	6.8888E-02
3.7300E+02	6.0230E+01	4.3656E+01	1.6574E+01	2.7518E-01

3.7300E+02	4.3633E+01	4.3656E+01	-2.3344E-02	5.3501E-04
3.7400E+02	4.8957E+01	4.7292E+01	1.6645E+00	3.3999E-02
3.7400E+02	7.2412E+01	4.7292E+01	2.5120E+01	3.4690E-01
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